Dressed molecules in an optical lattice

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Abstract. We present the theory of an atomic gas in an optical lattice near a Feshbach resonance. We derive from first principles a generalized Hubbard model, that incorporates all the relevant two-body physics exactly, except for the background atom-atom scattering. For most atoms the background interactions are negligible, but this is not true for ^{6}Li, which has an exceptionally large background scattering length near the experimentally relevant Feshbach resonance at 834 G. Therefore, we show how to include background atom-atom scattering by solving the on-site two-body Feshbach problem exactly. We apply the obtained solution to ^{6}Li and find that the background interactions indeed have a significant effect in this case.

1. Introduction.

The field of ultracold atoms has recently seen many exciting developments in which strong interactions play a crucial role. Examples are the observation of the quantum phase transition between the superfluid and the Mott-insulator phase of a Bose gas in an optical lattice [1], the observation of the BEC-BCS crossover in a Fermi gas [2, 3, 4, 5, 6, 7], and the observation of fermionization in an one-dimensional Bose gas [8, 9]. To a large extent these developments are due to the successful implementation of two new experimental techniques, namely the use of optical lattices [10] and the application of Feshbach resonances in the collision of two atoms [11, 12]. Both techniques have contributed greatly to the unprecendented control over the relevant physical parameters of an atomic gas.

In this article, we focus on the combination of these two important techniques and present the microscopic theory of an atomic gas in an optical lattice near a Feshbach resonance. This problem was already studied in ref. [13], where it was argued that an optical lattice could be very well suited to overcome the experimental difficulties in studying the quantum phase transition that occurs in an atomic Bose gas near a Feshbach resonance [14, 15]. The observation of this quantum Ising transition between a

phase with only a molecular condensate and a phase with both an atomic and a molecular condensate is complicated by the fast vibrational relaxation of the Feshbach molecules due to collisions, which appears to prevent the creation of a molecular condensate [16]. In an optical lattice with low filling fractions, collisions can essentially be neglected and this problem is expected to be much less severe. Furthermore, in a subsequent study, a resonantly-interacting Bose-Fermi mixture in an optical lattice was considered, which led to the prediction of another XY-like quantum phase transition, associated with the Bose-Einstein condensation of the bosons in the mixture [17].

In both studies [13, 17], a generalized Hubbard model was obtained by incorporating the relevant two-body physics exactly. As a result, simple mean-field techniques could be used to accurately describe the many-body physics of the atomic gas near the Feshbach resonance in the optical lattice. This approach led to some discussion [18, 19], which motivated us to rederive in this article the proposed generalized Hubbard model from first principles by means of a field-theoretical calculation. In this manner, the validity of the original approach is put on an even more rigorous basis.

Another aspect that we discuss in this article, is the effect of background atom-atom scattering on the Feshbach physics. This effect was not incorporated in the previously mentioned studies, since only systems with a small background scattering length were considered. However, for ^{6}Li, which has an exceptionally large background scattering length near the experimentally relevant Feshbach resonance at 834 G, the neglect of the background interactions is no longer allowed. In this article, we therefore show how to include the background atom-atom scattering by exactly solving the two-body Feshbach problem on a single site of the optical lattice. The exact knowledge of the two-body physics on a single site can then be directly incorporated into a generalized Hubbard model that describes the many-body physics of ^{6}Li in an optical lattice near a Feshbach resonance, in a similar manner as recently achieved for ^{40}K [20].

2. Effective atom-molecule theory.

In this section, we give an *ab initio* field-theoretical derivation of the effective atom-molecule theory that describes an atomic gas in an optical lattice near a Feshbach resonance. The theory is formulated in the tight-binding limit and incorporates all the relevant two-body physics exactly. If desired, this rather technical section can be omitted in a first reading of the article. To facilitate this, section 3 has been written in such a way that it stands on its own. There, we show how to solve analytically the two-channel Feshbach problem for two atoms on a single site including background atom-atom scattering. We also apply the obtained theory to ^{6}Li.

2.1. Effective action.

The quantity of interest in a quantum-field theory is the generating functional Z of all the Green's functions. This functional determines all the possible correlation functions

of the system. Specifically, let us consider the field theory for an atom-molecule gas that is described by the action $S[\psi_a^*, \psi_a, \psi_m^*, \psi_m]$, with ψ_a and ψ_m being the atomic and molecular fields, respectively. The generating functional in imaginary time is defined by

$$
\begin{aligned}
&Z[J_a^*, J_a, J_m^*, J_m] \\
&= \int d[\psi_a^*] \, d[\psi_a] \, d[\psi_m^*] \, d[\psi_m] \exp\left\{-\frac{1}{\hbar}S[\psi_a^*, \psi_a, \psi_m^*, \psi_m] + S_J\right\},
\end{aligned} \tag{1}
$$

where the source currents couple to the fields according to,

$$
\begin{aligned}
S_J = \int d\tau \int d\mathbf{x} \, [\psi_a^*(\mathbf{x}, \tau)J_a(\mathbf{x}, \tau) + J_a^*(\mathbf{x}, \tau)\psi_a(\mathbf{x}, \tau) \\
+\psi_m^*(\mathbf{x}, \tau)J_m(\mathbf{x}, \tau) + J_m^*(\mathbf{x}, \tau)\psi_m(\mathbf{x}, \tau)] \, .
\end{aligned} \tag{2}
$$

By taking functional derivatives of Z with respect to the currents we can calculate all the correlation functions of the theory.

Instead of working with Z we usually prefer to work with the generating functional W of all the connected Green's functions, which is related to Z through $Z = \exp(W)$. The functional derivatives of W with respect to the currents are the expectation values of the fields, i.e.,

$$
\frac{\delta W}{\delta J_a(\mathbf{x}, \tau)} = \langle\psi_a^*(\mathbf{x}, \tau)\rangle \equiv \phi_a^*(\mathbf{x}, \tau) \tag{3}
$$

$$
\frac{\delta W}{\delta J_m(\mathbf{x}, \tau)} = \langle\psi_m^*(\mathbf{x}, \tau)\rangle \equiv \phi_m^*(\mathbf{x}, \tau). \tag{4}
$$

Similar equations hold for the expectation values of the complex conjugated fields $\psi_a(\mathbf{x}, \tau)$ and $\psi_m(\mathbf{x}, \tau)$. Instead of using W, which only depends on the current sources, it is possible to define a functional Γ that depends explicitly on the fields $\phi_a(\mathbf{x}, \tau)$ and $\phi_m(\mathbf{x}, \tau)$, and which is related to W by means of a Legendre transformation, i.e.,

$$
\begin{aligned}
\Gamma[\phi_a^*, \phi_a, \phi_m^*, \phi_m] = &- W[J_a^*, J_a, J_m^*, J_m] \\
&+ \int d\tau \int d\mathbf{x} \, [\phi_a^*(\mathbf{x}, \tau)J_a(\mathbf{x}, \tau) + J_a^*(\mathbf{x}, \tau)\phi_a(\mathbf{x}, \tau) \\
&+ \phi_m^*(\mathbf{x}, \tau)J_m(\mathbf{x}, \tau) + J_m^*(\mathbf{x}, \tau)\phi_m(\mathbf{x}, \tau)] \, .
\end{aligned} \tag{5}
$$

The reason for defining this functional is that Γ is related to the exact effective action of the system through $S^{\text{eff}} = -\hbar\Gamma$. Technically, Γ is the generating functional of all one-particle irreducible vertex functions. In our case, the exact effective action for the atom-molecule theory can be written as

$$
\begin{aligned}
S^{\text{eff}}[\phi_a^*, \phi_a, \phi_m^*, \phi_m] = \text{Tr}\left[-\phi_a^*\hbar G_a^{-1}\phi_a - \phi_m^*\hbar G_m^{-1}\phi_m \right. \\
\left. + g\left(\phi_m^*\phi_a\phi_a + \phi_a^*\phi_a^*\phi_m\right) + \ldots\right],
\end{aligned} \tag{6}
$$

where $G_{a/m}$ is the exact propagator of the atoms/molecules, and g is the exact three-point vertex. The dots denote all possible other one-particle irreducible vertices, which turn out to be less relevant for our purposes.

2.2. Microscopic action.

Starting from the microscopic atom-molecule theory in an optical lattice, it is our goal to derive an effective quantum field theory, that contains the relevant two-body physics

exactly. For calculational convenience and to facilitate comparison with previous work [13], we consider the case of bosonic atoms. The generalization to fermionic atoms is then straightforward.

The total microscopic action S describing resonantly-interacting atoms in an optical lattice can be split up in three parts, namely a purely atomic part S_a, a purely molecular part S_m and a coupling between atoms and molecules S_{am},

$$S = S_a + S_m + S_{am}. \tag{7}$$

The purely atomic part S_a is given by

$$S_a = \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \psi_a^*(\mathbf{x}, \tau) \left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m_a} - \mu + V_0(\mathbf{x}) \right) \psi_a(\mathbf{x}, \tau)$$
$$+ \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \frac{4\pi a_{bg}\hbar^2}{m_a} \psi_a^*(\mathbf{x}, \tau)\psi_a^*(\mathbf{x}, \tau)\psi_a(\mathbf{x}, \tau)\psi_a(\mathbf{x}, \tau)\ , \tag{8}$$

with μ the chemical potential, m_a the atomic mass, a_{bg} the background scattering length and $V_0(\mathbf{x})$ the external periodic potential due to the optical lattice. In first instance, we neglect the background atom-atom scattering, since we are primarily interested in the resonant interactions between the atoms and the molecules. For most atoms, this is an accurate approximation. Furthermore, the same approximation was also used in previous work [13], with which we ultimately want to compare the following derivation. Finally, in section 3 we overcome this approximation and show how to include the effect of background atom-atom scattering.

The purely molecular action S_m is given by

$$S_m = \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \psi_m^*(\mathbf{x}, \tau) \left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{4m_a} + \delta_B - 2\mu + 2V_0(\mathbf{x}) \right) \psi_m(\mathbf{x}, \tau)\ . \tag{9}$$

where δ_B is the so-called bare detuning (see also section 3). The action S_{am} corresponding to the atom-molecule coupling that describes the formation of a bare molecule from two atoms and vice versa, is given by

$$S_{am} = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}'\ g(\mathbf{x} - \mathbf{x}') \{\psi_m^*((\mathbf{x} + \mathbf{x}')/2, \tau)\psi_a(\mathbf{x}', \tau)\ \psi_a(\mathbf{x}, \tau)$$
$$+ \psi_a^*(\mathbf{x}', \tau)\psi_a^*(\mathbf{x}, \tau)\psi_m((\mathbf{x} + \mathbf{x}')/2, \tau)\}\ , \tag{10}$$

where $g(\mathbf{x})$ denotes the atom-molecule coupling.

We can write the actions involving the atomic fields in a more convenient way as

$$S_a + S_{am} = -\frac{\hbar}{2} \int_0^{\hbar\beta} d\tau d\tau' \int d\mathbf{x} d\mathbf{x}'$$
$$\times \left(\psi_a^*(\mathbf{x}, \tau), \psi_a(\mathbf{x}, \tau) \right) \mathbf{G}^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') \begin{pmatrix} \psi_a(\mathbf{x}', \tau') \\ \psi_a^*(\mathbf{x}', \tau') \end{pmatrix}, \tag{11}$$

with $\mathbf{G}$ the 2×2 (Nambu space) Green's function matrix, given by

$$\mathbf{G}^{-1} = \mathbf{G}_a^{-1} - \mathbf{\Sigma} = \mathbf{G}_a^{-1} \left(1 - \mathbf{G}_a \mathbf{\Sigma} \right). \tag{12}$$

Here, the atomic Green's function matrix $\mathbf{G}_\mathrm{a}^{-1}$ has the following form

$$\mathbf{G}_\mathrm{a}^{-1} = \begin{bmatrix} G_\mathrm{a}^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') & 0 \\ 0 & G_\mathrm{a}^{-1}(\mathbf{x}',\tau';\mathbf{x},\tau) \end{bmatrix}, \tag{13}$$

where the atomic zeroth-order Green's function G_a satisfies

$$\left\{ \hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m_\mathrm{a}} + V_0(\mathbf{x}) - \mu \right\} G_\mathrm{a}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\hbar\delta(\tau-\tau')\delta(\mathbf{x}-\mathbf{x}'). \tag{14}$$

The self-energy matrix $\hbar\boldsymbol{\Sigma}$ is given by

$$\hbar\boldsymbol{\Sigma} = \begin{bmatrix} 0 & 2g(\mathbf{x}-\mathbf{x}')\psi_\mathrm{m}((\mathbf{x}+\mathbf{x}')/2,\tau) \\ 2g(\mathbf{x}-\mathbf{x}')\psi_\mathrm{m}^*((\mathbf{x}+\mathbf{x}')/2,\tau) & 0 \end{bmatrix}$$
$$\times \delta(\tau-\tau'). \tag{15}$$

From the microscopic atom-molecule action we can calculate the grand-canonical partition function Z as the functional integral

$$Z = \int d[\psi_\mathrm{a}^*]d[\psi_\mathrm{a}]d[\psi_\mathrm{m}^*]d[\psi_\mathrm{m}] \exp\left\{ -\frac{1}{\hbar}S[\psi_\mathrm{a}^*,\psi_\mathrm{a},\psi_\mathrm{m}^*,\psi_\mathrm{m}] \right\}. \tag{16}$$

Since the integral is Gaussian in the atomic fields, we can perform this integral exactly, giving

$$\begin{aligned} Z &= \int d[\psi_\mathrm{m}^*]d[\psi_\mathrm{m}] \exp\left\{ -\frac{1}{2}\mathrm{Tr}[\ln(-\mathbf{G}^{-1})] - \frac{1}{\hbar}S_\mathrm{m} \right\} \\ &= \int d[\psi_\mathrm{m}^*]d[\psi_\mathrm{m}] \exp\left\{ -\frac{1}{2}\mathrm{Tr}[\ln(-\mathbf{G}_\mathrm{a}^{-1})] - \frac{1}{2}\mathrm{Tr}[\ln(\mathbf{1}-\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma})] - \frac{1}{\hbar}S_\mathrm{m} \right\}, \end{aligned} \tag{17}$$

where the traces are taken over a 2×2 matrix structure, coordinate space, and imaginary time. By integrating out the atoms, we have obtained an effective action for the bare molecules that consists of three terms. The first term represents the contribution from the ideal atomic gas, which does not depend on the bare molecular fields. The second term can be brought in a more illuminating form by expanding the logarithm. Because of the trace, only even powers in the expansion give nonzero results, yielding

$$\frac{1}{2}\mathrm{Tr}[\ln(1-\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma})] = -\sum_{n=2,4,\dots} \frac{1}{2n}(\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma})^n. \tag{18}$$

The first nonzero term is of second order, namely $-\mathrm{Tr}\left[\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\right]/4$, and expresses that a molecule can break up into two atoms and recombine again. This term can be interpreted as corresponding to the self-energy of the bare molecules and a diagrammatic picture of the term is shown in figure 1. The higher-order terms in equation (18) pertain to interactions between the bare molecules.

2.3. Molecular self-energy.

Next, we evaluate the molecular self-energy term, $-\mathrm{Tr}\left[\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\right]/4$, by explicitly carrying out the trace. As a first step, we introduce center-of-mass coordinates
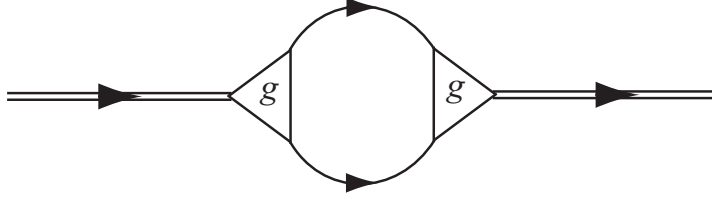
Figure 1. Diagrammatic representation of the term $-\mathrm{Tr}\left[\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\right]/4$, which expresses that a bare molecule can break up into two atoms and recombine again. The coupling strength between the atoms and the molecule is given by g. This diagram can be interpreted as a self-energy of the bare molecules.

$\mathbf{R} = (\mathbf{x}' + \mathbf{x}'')/2$, $\mathbf{R}' = (\mathbf{x} + \mathbf{x}''')/2$ and relative coordinates $\mathbf{r} = \mathbf{x}' - \mathbf{x}''$, $\mathbf{r}' = \mathbf{x}''' - \mathbf{x}$. Writing out the trace in these coordinates yields

$$
\begin{aligned}
-\frac{1}{4}\mathrm{Tr}\left[\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\mathbf{G}_\mathrm{a}\boldsymbol{\Sigma}\right] = & -\frac{2}{\hbar^2}\int_0^{\hbar\beta} d\tau\ d\tau' \int d\mathbf{R}\ d\mathbf{R}'\ d\mathbf{r}\ d\mathbf{r}'\ g(\mathbf{r})g(\mathbf{r}')\psi_\mathrm{m}^*(\mathbf{R},\tau) \\
& \times \psi_\mathrm{m}(\mathbf{R}',\tau')\ G_\mathrm{a}(\mathbf{R}'+\mathbf{r}'/2,\tau;\mathbf{R}+\mathbf{r}/2,\tau')G_\mathrm{a}(\mathbf{R}'-\mathbf{r}'/2,\tau;\mathbf{R}-\mathbf{r}/2,\tau') \\
= & -\frac{2g^2}{\hbar^2}\int_0^{\hbar\beta} d\tau\ d\tau' \int d\mathbf{R}\ d\mathbf{R}'\psi_\mathrm{m}^*(\mathbf{R},\tau)\psi_\mathrm{m}(\mathbf{R}',\tau') \\
& \times G_\mathrm{a}(\mathbf{R}',\tau;\mathbf{R},\tau')G_\mathrm{a}(\mathbf{R}',\tau;\mathbf{R},\tau'), \qquad (19)
\end{aligned}
$$

where in the last line we made use of the usual pseudopotential approximation $g(\mathbf{r}) = g\delta(\mathbf{r})$.

In order to proceed, we rewrite the atomic Green's functions by performing an expansion for both their spacial and temporal arguments. For the expansion of the space dependence, we use the complete set of atomic Bloch wave functions $\chi_{\mathbf{n},\mathbf{k}}^\mathrm{a}$, which are solutions to the Schrödinger equation for a particle in a periodic potential

$$
\left[-\frac{\hbar^2\nabla^2}{2m_\mathrm{a}} + V_0(\mathbf{x})\right]\chi_{\mathbf{n},\mathbf{k}}^\mathrm{a}(\mathbf{x}) = \epsilon_{\mathbf{n},\mathbf{k}}\chi_{\mathbf{n},\mathbf{k}}^\mathrm{a}(\mathbf{x}). \qquad (20)
$$

Here, the exact Bloch wave functions are given by

$$
\chi_{\mathbf{n},\mathbf{k}}^\mathrm{a}(\mathbf{x}) = \frac{1}{\sqrt{N_\mathrm{s}}}\sum_i e^{i\mathbf{k}\cdot\mathbf{x}_i}w_{\mathbf{n}}^\mathrm{a}(\mathbf{x}-\mathbf{x}_i), \qquad (21)
$$

with $w_{\mathbf{n}}^\mathrm{a}(\mathbf{x})$ the so-called (atomic) Wannier functions, $\mathbf{x}_i$ the location of the optical lattice sites, N_s the total number of sites, $\mathbf{k}$ the lattice momentum, and $\mathbf{n}$ a set of quantum numbers for the various Bloch bands in the optical lattice. The Fourier expansion in imaginary time is performed by using the well-known Matsubara modes [21]. Combining the two expansions, we obtain

$$
G_\mathrm{a}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{\hbar\beta}\sum_n\sum_{\mathbf{n},\mathbf{k}} G_\mathrm{a}(\mathbf{n},\mathbf{k};i\omega_n)\chi_{\mathbf{n},\mathbf{k}}(\mathbf{x})\chi_{\mathbf{n},\mathbf{k}}^*(\mathbf{x}')e^{-i\omega_n(\tau-\tau')}. \qquad (22)
$$

with ω_n the Matsubara frequencies and $G_\mathrm{a}(\mathbf{n},\mathbf{k};i\omega_n)$ given by

$$
G_\mathrm{a}(\mathbf{n},\mathbf{k};i\omega_n) = \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\mathbf{k}} - \mu}. \qquad (23)
$$

Next, we also expand the space and imaginary-time arguments of the molecular fields $\psi_{\mathrm{m}}(\mathbf{x}, \tau)$. For the temporal expansion we use again the Matsubara modes and for the spacial expansion we use the (molecular) Wannier functions $w_{\mathbf{n}}^{\mathrm{m}}(\mathbf{x})$. As a result,

$$\psi_{\mathrm{m}}(\mathbf{x}, \tau) = \frac{1}{\sqrt{\hbar\beta}} \sum_{n} \sum_{\mathbf{n},i} b_{\mathbf{n},i}(\omega_n) w_{\mathbf{n}}^{\mathrm{m}}(\mathbf{x} - \mathbf{x}_i) e^{-i\omega_n\tau}. \tag{24}$$

with the complex conjugated version for ψ_m^*. The operators $b_{\mathbf{n},i}$ annihilate a molecule with a set of quantum numbers $\mathbf{n}$ on site i of the lattice.

Substituting equations (22) and (24) into (19), yields

$$\begin{aligned}
-\frac{1}{4}\mathrm{Tr}\left[\mathbf{G}_{\mathrm{a}}\mathbf{\Sigma}\mathbf{G}_{\mathrm{a}}\mathbf{\Sigma}\right] = &-\frac{2g^2}{\hbar^5\beta^3} \sum_{n,n'} \sum_{m,m'} \sum_{i,j} \sum_{\mathbf{m},\mathbf{m}'} \sum_{\mathbf{n},\mathbf{n}'} \sum_{\mathbf{k},\mathbf{k}'} \int_0^{\hbar\beta} d\tau \; d\tau' \int d\mathbf{R} \; d\mathbf{R}' \\
&\times b_{\mathbf{m},i}^*(\omega_n) b_{\mathbf{m}',j}(\omega_{n'}) e^{i\omega_n\tau} e^{-i\omega_{n'}\tau'} e^{-i(\omega_m+\omega_{m'})(\tau-\tau')} \\
&\times w_{\mathbf{m}}^{\mathrm{m}*}(\mathbf{R} - \mathbf{x}_i) w_{\mathbf{m}'}^{\mathrm{m}}(\mathbf{R}' - \mathbf{x}_j) G_{\mathrm{a}}(\mathbf{n}, \mathbf{k}; i\omega_m) G_{\mathrm{a}}(\mathbf{n}', \mathbf{k}'; i\omega_{m'}) \\
&\times \chi_{\mathbf{n},\mathbf{k}}^{\mathrm{a}}(\mathbf{R}) \chi_{\mathbf{n},\mathbf{k}}^{\mathrm{a}*}(\mathbf{R}') \chi_{\mathbf{n}',\mathbf{k}'}^{\mathrm{a}}(\mathbf{R}) \chi_{\mathbf{n}',\mathbf{k}'}^{\mathrm{a}*}(\mathbf{R}').
\end{aligned} \tag{25}$$

The integrals over the imaginary time variables τ and τ' can now easily be performed, resulting in the conditions $\omega_n = \omega_{n'} = \omega_m + \omega_{m'}$. Furthermore, if the optical lattice is deep, it can at every site be well approximated by an harmonic potential, characterized by the frequency ω. Then, we are also allowed to use the so-called tight-binding limit, in which the Wannier functions $w_{\mathbf{n}}$ are replaced by the tight-binding functions $\phi_{\mathbf{n}}$, i.e.

$$w_{\mathbf{n}}(\mathbf{R} - \mathbf{x}_i) \simeq \phi_{\mathbf{n}}(\mathbf{R} - \mathbf{x}_i). \tag{26}$$

Here, $\phi_{\mathbf{n}}(\mathbf{R})$ are the eigenstates of the three-dimensional isotropic harmonic oscillator potential given in spherical coordinates by

$$\begin{aligned}
\phi_{\mathbf{n}}(\mathbf{R}) \equiv \phi_{n,\ell,m}(\mathbf{R}) = &\sqrt{\frac{2}{l^3}} \left(\begin{array}{c} n + \ell + 1/2 \\ n \end{array} \right)^{-1/2} \frac{1}{\sqrt{(\ell + 1/2)!}} \\
&\times e^{-R^2/2l^2} L_n^{(1/2+\ell)}((R/l)^2) \, (R/l)^\ell \, Y_{\ell m}(\theta, \phi),
\end{aligned} \tag{27}$$

where $L_n^{(1/2+\ell)}(X)$ are the generalized Laguerre polynomials and $Y_{\ell,m}(\theta, \phi)$ the spherical harmonics. For the atoms, the harmonic oscillator length l is given by $l_{\mathrm{a}} = \sqrt{\hbar/m_{\mathrm{a}}\omega}$; for the molecules, the harmonic oscillator length l is given by $l_{\mathrm{a}}/\sqrt{2}$. Furthermore, in the extreme tight-binding limit the energies $\epsilon_{\mathbf{n},\mathbf{k}}$ in equation (23) are given by $\epsilon_{\mathbf{n},\mathbf{k}} = \epsilon_{\mathbf{n}} = (2n + \ell + 3/2)\hbar\omega$ and only depend on the radial and angular momentum quantum numbers n and ℓ, respectively. Similarly, we have that $G_{\mathrm{a}}(\mathbf{n}, \mathbf{k}; i\omega_m) = G_{\mathrm{a}}(\mathbf{n}; i\omega_m)$. Also note that in the tight-binding limit, the overlap for wave functions on different lattice sites is negligible. As a result, we can consider only the terms on the right-hand side of equation (25) that have all atomic and molecular Wannier functions centered around the same site $\mathbf{x}_i$. Furthermore, because of translational invariance of the lattice, we can set $\mathbf{x}_i$ to zero in the integrant. As a result, the right-hand side of equation (25) does not depend on $\mathbf{k}, \mathbf{k}'$ anymore, and the sum over the lattice momenta yields the factor N_{s}^2.

Next, we evaluate the sum over Matsubara frequencies, keeping the external frequency $\omega_m + \omega_{m'} = \omega_n$ of the molecules fixed. First, we rewrite the product of Green's functions as

$$G_{\rm a}(\mathbf{n}, i\omega_m)G_{\rm a}(\mathbf{n}', i\omega_{m'}) = -\hbar \frac{G_{\rm a}(\mathbf{n}, i\omega_m) + G_{\rm a}(\mathbf{n}', i\omega_{m'})}{-i\hbar(\omega_m + \omega_{m'}) + \epsilon_\mathbf{n} + \epsilon_{\mathbf{n}'} - 2\mu}. \tag{28}$$

Subsequently, we perform the sum and take the two-body limit, which amounts to taking the atomic distribution functions, obtained after the Matsubara summation, equal to zero [21]. We find

$$-\frac{1}{4}\mathrm{Tr}\left[\mathbf{G}_{\rm a}\mathbf{\Sigma}\mathbf{G}_{\rm a}\mathbf{\Sigma}\right] = -\frac{2g^2}{\hbar}\sum_i \sum_n \sum_{\mathbf{m},\mathbf{m}'} \sum_{\mathbf{n},\mathbf{n}'} \int d\mathbf{R}\; d\mathbf{R}'\; b_{\mathbf{m},i}^*(\omega_n)b_{\mathbf{m}',i}(\omega_n)$$

$$\times \frac{\phi_\mathbf{m}^{{\rm m}*}(\mathbf{R})\phi_{\mathbf{m}'}^{\rm m}(\mathbf{R}')\phi_\mathbf{n}^{\rm a}(\mathbf{R})\phi_\mathbf{n}^{{\rm a}*}(\mathbf{R}')\phi_{\mathbf{n}'}^{\rm a}(\mathbf{R})\phi_{\mathbf{n}'}^{{\rm a}*}(\mathbf{R}')}{-i\hbar\omega_n + \epsilon_\mathbf{n} + \epsilon_{\mathbf{n}'} - 2\mu}, \tag{29}$$

where $\phi_\mathbf{n}^{{\rm m}/{\rm a}}(\mathbf{R})$ denotes the molecular/atomic tight-binding function. For systems of interest to us, the molecules occupy only the lowest Bloch band, i.e., we take the band indices $\mathbf{m}$ and $\mathbf{m}'$ of the molecular fields in the last expression equal to zero. The tight-binding function $\phi_\mathbf{0}^{\rm m}$ is given by $\phi_\mathbf{0}^{\rm m}(\mathbf{R}) = (2/\pi l_{\rm a}^2)^{3/4}\, e^{-(R/l_{\rm a})^2}$.

Next, we need to evaluate the integrals over $\mathbf{R}$ and $\mathbf{R}'$ of the form

$$\int d\mathbf{R}\phi_\mathbf{0}^{{\rm m}*}(\mathbf{R})\phi_\mathbf{n}^{\rm a}(\mathbf{R})\phi_{\mathbf{n}'}^{\rm a}(\mathbf{R}) = 2\left(\frac{2}{\pi l_{\rm a}^2}\right)^{3/4}$$

$$\times \int dR\; d\theta\; d\phi\; R^{2+\ell+\ell'}\sin\theta\; e^{-2R^2}\frac{L_n^{(1/2+\ell)}(R^2)}{\sqrt{(\ell+1/2)!}}\frac{L_{n'}^{(1/2+\ell')}(R^2)}{\sqrt{(\ell'+1/2)!}}$$

$$\times Y_{\ell m}(\theta,\phi)Y_{\ell'm'}(\theta,\phi)\left(\begin{array}{c} n+\ell+1/2 \\ n \end{array}\right)^{-1/2}\left(\begin{array}{c} n'+\ell'+1/2 \\ n' \end{array}\right)^{-1/2}, \tag{30}$$

where on the right-hand side of the above equation the integration variable R is made dimensionless using the length $l_{\rm a}$. The integrations over the angles can be directly evaluated using the orthonormality relations for the spherical harmonics. To evaluate the remaining integral over R, we make use of the following relation [22]

$$\int_0^\infty dX\; e^{-2X^2}X^{2+2\ell}L_n^{(1/2+\ell)}(X^2)L_{n'}^{(1/2+\ell)}(X^2)$$

$$= \frac{1}{2}\int_0^\infty dy\; e^{-2y}y^{1/2+\ell}L_n^{(1/2+\ell)}(y)L_{n'}^{(1/2+\ell)}(y)$$

$$= \frac{\Gamma(n+n'+\ell+3/2)}{2n!n'!}\frac{1}{2^{n+n'+\ell+3/2}}. \tag{31}$$

Using this, we find that equation (30) can be written as

$$\int d\mathbf{R}\phi_\mathbf{0}^{{\rm m}*}(\mathbf{R})\phi_\mathbf{n}^{\rm a}(\mathbf{R})\phi_{\mathbf{n}'}^{\rm a}(\mathbf{R}) = (-1)^m\delta_{-m,m'}\left(\frac{2}{\pi l_{\rm a}^2}\right)^{3/4}\frac{\Gamma(n+n'+\ell+3/2)}{n!n'!}$$

$$\times \frac{1}{2^{n+n'+\ell+3/2}}\frac{1}{(\ell+1/2)!}\left(\begin{array}{c} n+\ell+1/2 \\ n \end{array}\right)^{-1/2}\left(\begin{array}{c} n'+\ell+1/2 \\ n' \end{array}\right)^{-1/2}. \tag{32}$$

Finally, we have to perform the sum over the quantum numbers of equation (32). We first partially evaluate the resulting sum over the quantum numbers $\mathbf{n}$ and $\mathbf{n}'$ by summing

out all the contributions that have the same energy $\epsilon_q \equiv \epsilon_{q,0} = \epsilon_{n,\ell} + \epsilon_{n',\ell} - 3\hbar\omega/2$. This yields

$$\sum_{\mathbf{n},\mathbf{n}'} \left[\int d\mathbf{R} \phi_{\mathbf{0}}^{\mathrm{m}*}(\mathbf{R}) \phi_{\mathbf{n}}^{\mathrm{a}}(\mathbf{R}) \phi_{\mathbf{n}'}^{\mathrm{a}}(\mathbf{R}) \right]^2 \delta_{q,n+n'+\ell} = \phi_q^{\mathrm{aa}*}(\mathbf{0}) \phi_q^{\mathrm{aa}}(\mathbf{0}), \tag{33}$$

where the relative wavefunctions of two particles in a harmonic potential $\phi_q^{\mathrm{aa}}(\mathbf{r})$ will be introduced in section 3 and are given by equation (55). The reason for expressing the sum in terms of the relative wavefunctions $\phi_q^{\mathrm{aa}}(\mathbf{r})$ is to reveal the complete agreement between the field-theoretical calculation in this section and the two-body calculations in section 3.

For the second order term corresponding to the molecular self-energy we now obtain

$$-\frac{1}{4} \mathrm{Tr}\left[\mathbf{G}_{\mathrm{a}} \boldsymbol{\Sigma} \mathbf{G}_{\mathrm{a}} \boldsymbol{\Sigma} \right] = -2g^2 \sum_{i,n} b_{\mathbf{0},i}^*(\omega_n) b_{\mathbf{0},i}(\omega_n)$$

$$\times \sum_q \frac{\phi_q^{\mathrm{aa}*}(\mathbf{0}) \phi_q^{\mathrm{aa}}(\mathbf{0})}{-i\hbar\omega_n + \epsilon_q + 3\hbar\omega/2 - 2\mu}. \tag{34}$$

This sum contains an ultraviolet divergence resulting from the use of pseudopotentials. In section 3, we show how to deal with this divergence by means of a renormalization procedure, which leads to the final form of the molecular self-energy $\hbar\Sigma_{\mathrm{m}}$

$$\hbar\Sigma_{\mathrm{m}}(i\hbar\omega_n) = g^2 \frac{\Upsilon(i\hbar\omega_n - 3\hbar\omega/2 + 2\mu)}{\sqrt{2}\pi l_{\mathrm{a}}^3 \hbar\omega}, \tag{35}$$

where $\Upsilon(z)$ is the ratio of two gamma functions

$$\Upsilon(z) \equiv \frac{\Gamma(-z/2\hbar\omega + 3/4)}{\Gamma(-z/2\hbar\omega + 1/4)}. \tag{36}$$

Note that the self-energy of equation (35) is completely equivalent to the self-energy obtained from a two-body calculation in ref. [13].

2.4. Generalized Hubbard model

So far, we have calculated the self-energy of the bare molecules, but we have not yet taken into account the effects due to the purely molecular action S_{m} and the purely atomic action S_{a}. This is what we do next.

The purely action S_{m}, given by equation (9), can be rewritten by using equation (24), which yields

$$S_{\mathrm{m}} = \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \psi_{\mathrm{m}}^*(\mathbf{x},\tau) \left(\hbar\partial_\tau - \frac{\hbar^2 \nabla^2}{4m_{\mathrm{a}}} + \delta_{\mathrm{B}} - 2\mu + 2V_0(\mathbf{x}) \right) \psi_{\mathrm{m}}(\mathbf{x},\tau)$$

$$= \sum_n \sum_{i,j} \sum_{\mathbf{m},\mathbf{m}'} b_{\mathbf{m},i}^*(\omega_n) b_{\mathbf{m}',j}(\omega_n) \int d\mathbf{x}\, w_{\mathbf{m}}^{\mathrm{m}*}(\mathbf{x}-\mathbf{x}_i)$$

$$\times \left(-i\hbar\omega_n - \frac{\hbar^2 \nabla^2}{4m_{\mathrm{a}}} + 2V_0(\mathbf{x}) + \delta_{\mathrm{B}} - 2\mu \right) w_{\mathbf{m}'}^{\mathrm{m}}(\mathbf{x}-\mathbf{x}_j), \tag{37}$$

From which we can immediately read off the hopping term t_{m} and the on-site energy ϵ_{m}. For our purposes, the important case is when the molecules are in the lowest band.

Then, we find for the hopping parameter t_{m}

$$t_{\mathrm{m}} = -\int d\mathbf{x}\; w_{\mathbf{0}}^{\mathrm{m}*}(\mathbf{x} - \mathbf{x}_i) \left[-\frac{\hbar^2 \nabla^2}{4m_{\mathrm{a}}} + 2V_0(\mathbf{x}) \right] w_{\mathbf{0}}^{\mathrm{m}}(\mathbf{x} - \mathbf{x}_j), \tag{38}$$

where i and j are nearest-neighbouring sites. The on-site energy ϵ_{m} is given by

$$\epsilon_{\mathrm{m}} = \int d\mathbf{x}\; w_{\mathbf{0}}^{\mathrm{m}*}(\mathbf{x} - \mathbf{x}_i) \left[-\frac{\hbar^2 \nabla^2}{4m_{\mathrm{a}}} + 2V_0(\mathbf{x}) \right] w_{\mathbf{0}}^{\mathrm{m}}(\mathbf{x} - \mathbf{x}_i). \tag{39}$$

As a result, the action S_{m} can be written as a lattice action

$$S_{\mathrm{m}} = \sum_n \left\{ -t_{\mathrm{m}} \sum_{\langle i,j \rangle} b_i^*(\omega_n) b_j(\omega_n) \right.$$
$$\left. + \sum_i \left(-i\hbar\omega_n + \epsilon_{\mathrm{m}} + \delta_{\mathrm{B}} - 2\mu \right) b_i^*(\omega_n) b_i(\omega_n) \right\}, \tag{40}$$

where $\langle i,j \rangle$ denotes the sum over nearest neighbours and $\epsilon_{\mathrm{m}} = 3\hbar\omega/2$ in the tight-binding limit.

In exactly the same way, we can rewrite the atomic action S_{a} for the lowest Bloch band, yielding

$$S_{\mathrm{a}} = \sum_n \left\{ -t_{\mathrm{a}} \sum_{\langle i,j \rangle} a_i^*(\omega_n) a_j(\omega_n) \right.$$
$$\left. + \sum_i \left(-i\hbar\omega_n + \epsilon_{\mathrm{a}} - \mu \right) a_i^*(\omega_n) a_i(\omega_n) \right\}, \tag{41}$$

with the atomic hopping parameter t_{a} given by

$$t_{\mathrm{a}} = -\int d\mathbf{x}\; w_{\mathbf{0}}^{\mathrm{a}*}(\mathbf{x} - \mathbf{x}_i) \left[-\frac{\hbar^2 \nabla^2}{2m_{\mathrm{a}}} + V_0(\mathbf{x}) \right] w_{\mathbf{0}}^{\mathrm{a}}(\mathbf{x} - \mathbf{x}_j), \tag{42}$$

where i and j are nearest-neighbouring sites. For the on-site energy ϵ_{a} we find

$$\epsilon_{\mathrm{a}} = \int d\mathbf{x}\; w_{\mathbf{0}}^{\mathrm{a}*}(\mathbf{x} - \mathbf{x}_i) \left[-\frac{\hbar^2 \nabla^2}{2m_{\mathrm{a}}} + V_0(\mathbf{x}) \right] w_{\mathbf{0}}^{\mathrm{a}}(\mathbf{x} - \mathbf{x}_i). \tag{43}$$

The hopping parameters $t_{\mathrm{a,m}}$ satisfy exactly the relation [20]

$$t_{\mathrm{a,m}} = \frac{\hbar\omega\lambda}{\pi^{3/2} l_{\mathrm{a,m}}}\; e^{-(\lambda/\sqrt{2}\pi l_{\mathrm{a,m}})^2} \tag{44}$$

with λ the wavelength of the lattice laser and $l_{\mathrm{m}} = l_{\mathrm{a}}/\sqrt{2}$. Furthermore, in the tight-binding limit, $\epsilon_{\mathrm{a}} = 3\hbar\omega/2$.

Combining equations (34), (35) and (40), we find that the on-site bare molecular propagator is given by

$$-\hbar G_{\mathrm{m}}^{-1}(i\hbar\omega_n) = -i\hbar\omega_n + 3\hbar\omega/2 - 2\mu + \delta + \hbar\Sigma_m(i\hbar\omega_n). \tag{45}$$

with δ the renormalized detuning (see section 3). We perform an analytic continuation $i\hbar\omega_n \to E + i0$ and the zeros of the above equation are the poles of the Green's function,

which in turn correspond to the physical eigenstates of the on-site problem. To study these eigenstates, we calculate the spectral weight function $\rho(E)$, given by

$$\rho(E) = -\frac{1}{\pi\hbar}\text{Im}\left[G_\text{m}^{(+)}(E)\right], \tag{46}$$

where $G_\text{m}^{(+)}(E)$ is the retarded Green's function of the system, i.e., $G_\text{m}^{(+)}(E) = G_\text{m}(E+i0)$. In the two-body limit the chemical potential is zero and, because the self-energy is real, the spectral weight function becomes a set of delta functions located at the solutions ϵ_σ of the equation

$$\frac{3}{2}\hbar\omega + \delta = \epsilon_\sigma - g^2\left[\frac{\Upsilon(\epsilon_\sigma - 3\hbar\omega/2)}{\sqrt{2}\pi l_\text{a}^3\hbar\omega}\right], \tag{47}$$

where we note that the delta functions have strength Z_σ, given by

$$Z_\sigma = \left(1 - \left.\frac{\partial\hbar\Sigma_\text{m}(E)}{\partial E}\right|_{E=\epsilon_\sigma}\right)^{-1}. \tag{48}$$

We now have all ingredients needed for the effective atom-molecule theory, since we can substitute G_a^{-1} and G_m^{-1} and g in equation (6). In this manner, we have incorporated the on-site two-body physics exactly in the effective many-body theory. Furthermore, from the derived expression for the on-site bare molecular Green's function, we introduce the convenient notion of dressed molecular fields b_σ, by making use of

$$-\langle bb^*\rangle \equiv G_\text{m}(i\hbar\omega_n) = \sum_\sigma Z_\sigma \frac{-\hbar}{-i\hbar\omega_n + \epsilon_\sigma - 2\mu} \equiv -\sum_\sigma Z_\sigma\langle b_\sigma b_\sigma^*\rangle. \tag{49}$$

Using these dressed molecular fields, we finally find the Hamiltonian representation of our effective action, given by

$$\begin{aligned}
H = & -t_\text{a}\sum_{\langle i,j\rangle} a_i^\dagger a_j - t_m\sum_\sigma\sum_{\langle i,j\rangle} b_{i,\sigma}^\dagger b_{j,\sigma} \\
& + \sum_\sigma\sum_i (\epsilon_\sigma - 2\mu)\, b_{i,\sigma}^\dagger b_{i,\sigma} + \sum_i(\epsilon_\text{a} - \mu)a_i^\dagger a_i \\
& + g'\sum_\sigma\sum_i \sqrt{Z_\sigma}\left(b_{i,\sigma}^\dagger a_i a_i + a_i^\dagger a_i^\dagger b_{i,\sigma}\right),
\end{aligned} \tag{50}$$

where $\langle i,j\rangle$ denotes a sum over nearest-neighboring sites, $a_i^\dagger/a_i$ denote the creation/annihilation operators of a single atom at site i, $b_{i,\sigma}^\dagger/b_{i,\sigma}$ denote the creation/annihilation operators corresponding to the dressed molecular fields at site i, and the effective atom-molecule coupling in the optical lattice is given by

$$g' = g\int d\mathbf{x}\left[\phi_\mathbf{0}^\text{m*}(\mathbf{x})\phi_\mathbf{0}^\text{a}(\mathbf{x})\phi_\mathbf{0}^\text{a}(\mathbf{x})\right]. \tag{51}$$

From equation (50), we see that the effective Hamiltonian depends on several parameters. In particular, it depends on the energies of the dressed molecular fields ϵ_σ and the wavefunction renormalization factors Z_σ. In this section, we calculated these parameters from first principles by a field-theoretical calculation. But from a comparison with ref. [13], we see that exactly the same results can be obtained from just a two-body calculation on a single site. This is as expected, since the poles of the molecular

Green's function correspond to the physical eigenstates of the on-site two-body Feshbach problem.

So far, we did not take into account background atom-atom scattering, which is expected to be of particular importance for ^{6}Li, which has an extremely large background scattering length. Because we use an effective Hamiltonian and dressed molecular fields, we can include the background scattering in a very convenient way. Namely, if we are able to solve the two-body physics on a single site including background scattering, then, through the notion of our dressed fields, the background scattering gets automatically incorporated into the many-body theory. This is what we achieve in the next section.

3. Two-body physics on a single site.

Consider the Feshbach problem for two atoms on a single site of an optical lattice. In the typical case of experimental interest, the optical lattice potential is deep and the energy of the atoms is low. As a result, the on-site potential is well approximated by an isotropic harmonic potential with angular frequency ω. Furthermore, the atoms interact with each other through the potential V_{aa} which depends only on their relative coordinate $\mathbf{r}$, while the atom-molecule coupling is given by V_{am}. The resulting problem can be separated into a center-of-mass part and a relative part. Only the relative part is important in solving the two-body physics on a single site, while the center-of-mass part determines the tunneling of molecules between adjacent sites.

Taking all this into account, the relative Schrödinger equation for the two-channel Feshbach problem on a single site becomes

$$\begin{pmatrix} H_0 + V_{\mathrm{aa}} & V_{\mathrm{am}} \\ V_{\mathrm{am}} & \delta_{\mathrm{B}} \end{pmatrix} \begin{pmatrix} |\psi_{\mathrm{aa}}\rangle \\ |\psi_{\mathrm{m}}\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_{\mathrm{aa}}\rangle \\ |\psi_{\mathrm{m}}\rangle \end{pmatrix}, \tag{52}$$

where δ_{B} denotes the energy of the bare molecular state and the relative noninteracting atomic Hamiltonian H_0 is given by

$$H_0 = -\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{m_{\mathrm{a}}} + \frac{1}{4} m_{\mathrm{a}} \omega^2 \mathbf{r}^2. \tag{53}$$

Note that in writing down equation (52) we have assumed that the energy of the bare molecular state $|\psi_m\rangle$ is not affected by the optical lattice. This is well justified, since the spatial extent of the bare molecular wavefunction, centered around $\mathbf{r} = 0$, is very small compared the the harmonic oscillator length $l_{\mathrm{a}} \equiv \sqrt{\hbar/m_{\mathrm{a}}\omega}$. Furthermore, we can rewrite equation (52) to obtain the following equation for the energy eigenvalues

$$\langle \psi_{\mathrm{m}} | V_{\mathrm{am}} \frac{1}{E - H_0 - V_{\mathrm{aa}}} V_{\mathrm{am}} | \psi_{\mathrm{m}} \rangle = E - \delta_{\mathrm{B}}. \tag{54}$$

3.1. No background atom-atom scattering.

For many atoms of interest, such as for example rubidium or potassium, we have that $|V_{\mathrm{aa}}| \ll \hbar\omega$, which means that we can neglect V_{aa} compared to H_0. The resulting problem was solved in ref. [13] and here we will highlight the most important results.

The eigenfunctions of H_0 can be written in terms of the generalized Laguerre polynomials

$$\phi_n^{\mathrm{aa}}(r) = \langle \mathbf{r}|\phi_n^{\mathrm{aa}}\rangle = \frac{e^{-r^2/4l_{\mathrm{a}}^2}L_n^{1/2}(r^2/2l_{\mathrm{a}}^2)}{(2\pi l_{\mathrm{a}}^2)^{3/4}\sqrt{L_n^{1/2}(0)}}, \tag{55}$$

which correspond to the eigenenergies

$$E_n = (2n + 3/2)\hbar\omega, \tag{56}$$

for $n = 0, 1, 2, ...$ Using the completeness relation of the eigenfunctions $|\phi_n^{\mathrm{aa}}\rangle$, equation (54) can be rewritten as

$$\sum_n \frac{|\langle \psi_{\mathrm{m}}|V_{\mathrm{am}}|\phi_n^{\mathrm{aa}}\rangle|^2}{E - E_n} = E - \delta_{\mathrm{B}}. \tag{57}$$

Invoking the pseudopotential approxiation for fermions, which means that $\langle \mathbf{r}|V_{\mathrm{am}}|\psi_{\mathrm{m}}\rangle = g\delta(\mathbf{r})$, yields

$$E - \delta_{\mathrm{B}} = g^2 \sum_n \frac{\phi_n^{\mathrm{aa}*}(0)\phi_n^{\mathrm{aa}}(0)}{E - E_n}$$
$$= g^2 \left[\frac{\Upsilon(E)}{2\sqrt{2}\pi l_{\mathrm{a}}^3\hbar\omega} - \lim_{r\to 0}\frac{m}{4\pi\hbar^2 r} \right], \tag{58}$$

where the function $\Upsilon(E)$ was introduced in equation (36). The energy-independent divergence in equation (58) is an ultraviolet divergence resulting from the use of pseudopotentials, and was first obtained by Busch *et al.* in the context of a single-channel problem [23]. It can be dealt with by the following renormalization procedure. We define the renormalized detuning δ as

$$\delta \equiv \delta_{\mathrm{B}} - \lim_{r\to 0}\frac{m_{\mathrm{a}}g^2}{4\pi\hbar^2 r}, \tag{59}$$

which has two major advantages. Not only do we absorb the ultraviolet divergence in the definition of δ, but this renormalized detuning also has a relevant experimental meaning, in contrast to δ_{B}. Namely, δ corresponds to the detuning from the magnetic field B_0, at which the Feshbach resonance takes place in the absence of an optical lattice. This can be understood from the treatment of the homogeneous Feshbach problem without an optical lattice [24]. Here, the condition for the location of the Feshbach resonance is that the dressed molecular energy is equal to the threshold of the atomic continuum. This leads to the resonance condition $\delta_B = \lim_{r\to 0} m_{\mathrm{a}}g^2/4\pi\hbar^2 r$. As a result, the definition in equation (59) places the resonance in the absence of an optical lattice conveniently at $\delta = 0$ and, by construction, the (renormalized) detuning is of the following form

$$\delta(B) = \Delta\mu(B - B_0), \tag{60}$$

where $\Delta\mu$ is the difference in magnetic moment between the atoms in the open channel and the bare molecule in the closed channel.

Substituting equation (59) in equation (58) gives

$$E - \delta = \frac{g^2\Upsilon(E)}{2\sqrt{2}\pi l_{\mathrm{a}}^3\hbar\omega}, \tag{61}$$

which allows us to calculate the eigenenergies of the Feshbach problem on a single site given a certain detuning δ. Note the similarity between equation (61) and equation (47). The only two differences are a constant shift in the energy of $3\hbar\omega/2$ and a factor of 2, which are both readily explained. The shift of $3\hbar\omega/2$ is just the center-of-mass energy neglected in this relative calculation. The factor of 2 is due to the fact that here we consider fermions, while in the previous section we considered bosons. Since equations (47) and (61) are for the rest completely equivalent, we see that indeed the energies ϵ_σ of the dressed molecular fields b_σ, needed for the effective Hamiltonian of equation (50), can just as well be determined from a two-body calculation, as from a field-theoretical calculation. An obvious advantage of the two-body approach is that it is much simpler. Furthermore, as we show in the next paragraph, the two-body approach also allows for an incorporation of atom-atom scattering effects, which is of course also possible, but much more difficult from a field-theoretical point of view. These effects are particularly important for the fermion ^{6}Li, which has a very large background atom-atom scattering length a_{bg} near the extremely broad Feshbach resonance at $B_0 = 834$ G, namely on the order of $-1500a_0$, where a_0 is the Bohr radius.

3.2. With background atom-atom interaction.

The relative Schrödinger equation for two atoms in a harmonic potential interacting through the pseudopential $V_{\mathrm{aa}} = V_0\delta(\mathbf{r})$ without coupling to a molecular state

$$(H_0 + V_{\mathrm{aa}})|\phi_\nu\rangle = E_\nu|\phi_\nu\rangle \tag{62}$$

can be solved analytically for s-wave scattering following a treatment along the lines of ref. [23]. We just note that in this reference a suspicious 'molecular' bound state appears, which we believe to be unphysical for several reasons. Most convincing is probably to consider the limit $a_{\mathrm{bg}} \to 0^+$, in which case the interaction vanishes and we should recover the case of a simple harmonic oscillator. This is indeed what happens in ref. [23], except for the suspicious bound state, whose energy goes to minus infinity. Since such a state does not arise in the treatment of the harmonic oscillator, we conclude that the state is unphysical and we will exclude it from further calculations. Note also that for the specific case of ^{6}Li this issue is not relevant, since the suspicious state only occurs for positive values of a_{bg}.

The eigenvalues of equation (62) are given by $E_\nu = (2\nu + 3/2)\hbar\omega$, which are the solutions to the equation

$$\sqrt{2}\frac{\Gamma(-E_\nu/2\hbar\omega + 3/4)}{\Gamma(-E_\nu/2\hbar\omega + 1/4)} = \frac{l_{\mathrm{a}}}{a_{\mathrm{bg}}}, \tag{63}$$

where ν is in general not an integer. The corresponding eigenfunctions $\phi_\nu^{\mathrm{aa}}(r) = \langle r|\phi_\nu^{\mathrm{aa}}\rangle$ have the following form

$$\phi_\nu^{\mathrm{aa}}(r) = A_\nu e^{-r^2/4l_{\mathrm{a}}^2}\Gamma(-\nu)U(-\nu, 3/2, r^2/2l_{\mathrm{a}}^2), \tag{64}$$

where A_ν is a normalization constant and $U(-\nu, 3/2, r^2/2l^2)$ is a so-called confluent hypergeometric function of the second kind. We can determine A_ν by applying a limiting procedure to theorem 7.622 of ref. [22], resulting in

$$A_\nu^2 = \frac{\Gamma(-\nu - 1/2)}{4\sqrt{2}\pi^2 l_a^3 \Gamma(-\nu)[\psi^0(-\nu) - \psi^0(-\nu - 1/2)]}, \tag{65}$$

in which ψ^0 denotes the digamma function. Furthermore, we can use the completeness relation of the eigenfunctions $|\phi_\nu^{aa}\rangle$ to rewrite equation (54), which yields

$$\sum_\nu \frac{|\langle \psi_m | V_{am} | \phi_\nu^{aa} \rangle|^2}{E - E_\nu} = E - \delta_B. \tag{66}$$

In order to proceed from equation (66), we realize that the integral $\langle \psi_m | V_{am} | \phi_\nu^{aa} \rangle$ only acquires a finite contribution from a very small region around $\mathbf{r} = 0$, because the spatial extent of both the molecular wavefunction ψ_m and the atom-molecule coupling V_{am} is very small. This means that we are only interested in $\phi_\nu^{aa}(r)$ for small values of r, giving

$$\phi_\nu^{aa}(r) = -\sqrt{\pi} A_\nu \left(\frac{2\Gamma(-\nu)}{\Gamma(-\nu - 1/2)} - \sqrt{2}\frac{l_a}{r} + \mathcal{O}\left(\frac{r}{l_a}\right) \right)$$
$$= -\sqrt{2\pi} l_a A_\nu \left(\frac{1}{a_{bg}} - \frac{1}{r} + \mathcal{O}\left(\frac{r}{l_a^2}\right) \right), \tag{67}$$

where in the second line we used equation (63). Note that the eigenfunctions $\phi_\nu^{aa}(r)$ behave for small r completely analogous to the s-wave scattering states in the absence of an optical lattice $\psi_k(r)$, which are of the following form

$$\psi_k(r) = \frac{\sin[kr + \delta_0(k)]}{kr}, \tag{68}$$

where k is the relative momentum of the scattering state and $\delta_0(k)$ is the so-called s-wave phase shift, given by

$$k = \sqrt{\frac{m_a E_\nu}{\hbar^2}}, \tag{69}$$

$$\delta_0(k) = \tan^{-1}(-ka_{bg}). \tag{70}$$

Indeed, for small r, we have

$$\psi_k(r) = \cos\delta_0(k) + \frac{\sin\delta_0(k)}{kr} + \mathcal{O}(kr)$$
$$= -\frac{\sin\delta_0(k)}{k}\left(\frac{1}{a_{bg}} - \frac{1}{r} + \mathcal{O}(k^2 r) \right), \tag{71}$$

where in the second line we used equation (70). As a result, for small r

$$\phi_\nu^{aa}(r) = \sqrt{2\pi}\frac{kl_a A_\nu}{\sin\delta_0(k)}\psi_k(r). \tag{72}$$

This relation is illustrated by figure 2, where ϕ_ν^{aa}, $\psi_k' \equiv \sqrt{2\pi}kl_a A_\nu \psi_k / \sin\delta_0$ and their difference are plotted as a function of r. We see that the difference indeed vanishes for small r and increases with increasing r. The scattering states $\psi_k(r)$ are the solutions of
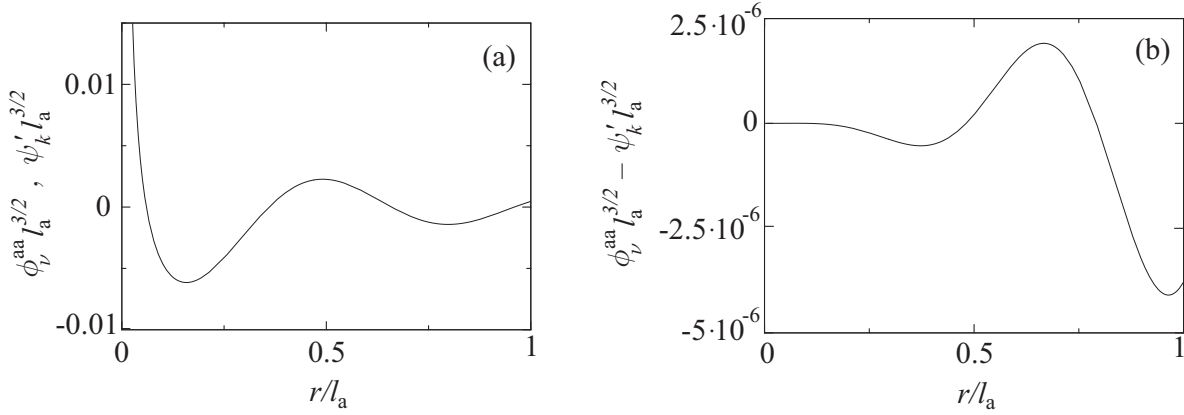
Figure 2. (a) Plot of the wavefunctions ϕ_ν^{aa} and ψ_k' as a function of the interatomic distance r. On the scale of the figure, the two wavefunctions cannot be distuinguished. (b) Plot of the difference between the wavefunctions ϕ_ν^{aa} and ψ_k' as a function of the interatomic distance r. Note that this difference is extremely small compared to the value of the wavefunctions themselves. All quantities on the axes are made dimensionless using the atomic harmonic oscillator length l_a

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the relative two-atom s-wave scattering problem without optical lattice and without atom-molecule coupling [24]. The physical reason for the similarity between $\phi_\nu(r)$ and $\psi_k(r)$ near $r = 0$ is due to the following: for small r compared to l_a, the atoms experience an effectively constant harmonic potential by which they are not affected. Therefore, for small r the wavefunction from the theory with optical lattice should, up to a normalization, reduce to the wavefunction from the theory without optical lattice. Since it is known how to solve the homogeneous Feshbach problem without an optical lattice [24], we are able to profit from this knowledge. This is what we do in the next paragraph.

3.3. Solving the two-atom Feshbach-problem.

By combining equations (66) and (72), we obtain

$$\sum_\nu \frac{2\pi k^2 l_a^2 A_\nu^2}{\sin^2 \delta_0(k)} \frac{|\langle \psi_m | V_{am} | \psi_k \rangle|^2}{E - E_\nu} = E - \delta_B. \tag{73}$$

From ref. [24], we have that

$$\langle \psi_m | V_{am} | \psi_k \rangle = \frac{g}{1 - i a_{bg} k}. \tag{74}$$

Substituting equations (65) and (74) into equation (73) and rewriting the result with the use of equation (70) yields

$$\frac{g^2}{2\pi a_{bg} l_a^2} \sum_\nu \frac{1}{[E - (2\nu + 3/2)] [\psi^0(-\nu) - \psi^0(-\nu - 1/2)]} = E - \delta_B. \tag{75}$$

Just like in section 3.1, we would like to renormalize the bare detuning δ_B, which has no experimental meaning, to the renormalized detuning δ, which gives the detuning

from the magnetic field B_0 at which the Feshbach resonance takes place in the absence of an optical lattice. From the homogeneous theory that takes a_{bg} into account [24], we find at resonance that

$$\delta_{\mathrm{B}} = \frac{g^2 m_{\mathrm{a}}}{4\pi\hbar^2 |a_{\mathrm{bg}}|}. \tag{76}$$

Defining the renormalized detuning δ as $\delta \equiv \delta_B - g^2 m_{\mathrm{a}}/4\pi\hbar^2|a_{\mathrm{bg}}|$ places the Feshbach resonance in the absence of an optical lattice conveniently at $\delta = 0$ and brings equation (75) into its final form

$$E - \delta = \frac{g^2}{2\pi a_{\mathrm{bg}} l_{\mathrm{a}}^2} \sum_\nu \frac{1}{[E - (2\nu + 3/2)]\,[\psi^0(-\nu) - \psi^0(-\nu - 1/2)]}$$
$$+ \frac{g^2 m_{\mathrm{a}}}{4\pi\hbar^2 |a_{\mathrm{bg}}|}, \tag{77}$$

where by construction $\delta = \Delta\mu(B - B_0)$ again. As in section 3.1, the term on the right-hand side of equation (77) can be interpreted as a molecular self-energy $\hbar\Sigma_{\mathrm{m}}(E)$. Furthermore, upon going to a many-body theory, the solutions of equation (77) can be interpreted as the energies ϵ_σ of the dressed molecular fields b_σ, resulting in a generalized Hubbard Hamiltonian in the same way as before.

For ^{6}Li, which has a very large a_{bg}, we expect the effects of the background scattering to be of particular importance. Therefore, in the next paragraph, we study equation (77) for the specific case of ^{6}Li to see if it leads to significant differences from the results given by equation (61), which doesn't take background scattering into account.

3.4. Lithium

Figure 3a shows the energy-levels of two interacting ^{6}Li atoms in the hyperfine states $|1\rangle$ and $|2\rangle$ on a single site near the Feshbach resonance at 834 G. The diagram has been obtained by numerically solving equation (77), where we used the known experimental values for $g(B)$ and $a_{\mathrm{bg}}(B)$ corresponding to ^{6}Li [25]. Note that for the extremely broad Feshbach resonance at 834 G these parameters depend on the magnetic field B. Furthermore, we took for l_{a} the realistic value 10^{-7} m, corresponding to $\omega = 10^6$ s^{-1}. In figure 3b the same diagram is shown, but this time without taking the background atom-atom scattering into account. This diagram has been obtained by numerically solving equation (61), where again the experimental value of the parameter $g(B)$, corresponding to ^{6}Li, was substituted.

From figure 3, we see that for ^{6}Li near the Feshbach resonance at 834 G it is important to include background atom-atom interactions, since it leads to a significant adjustment of the corresponding two-body energy-level diagram. Upon inclusion of the background atom-atom interactions, the horizontal asymptotes are shifted to different energy values and the avoided crossings, see also ref. [13], become much less broad. Physically, this is a result of the fact that the large value of a_{bg} effectively reduces the atom-molecule coupling.
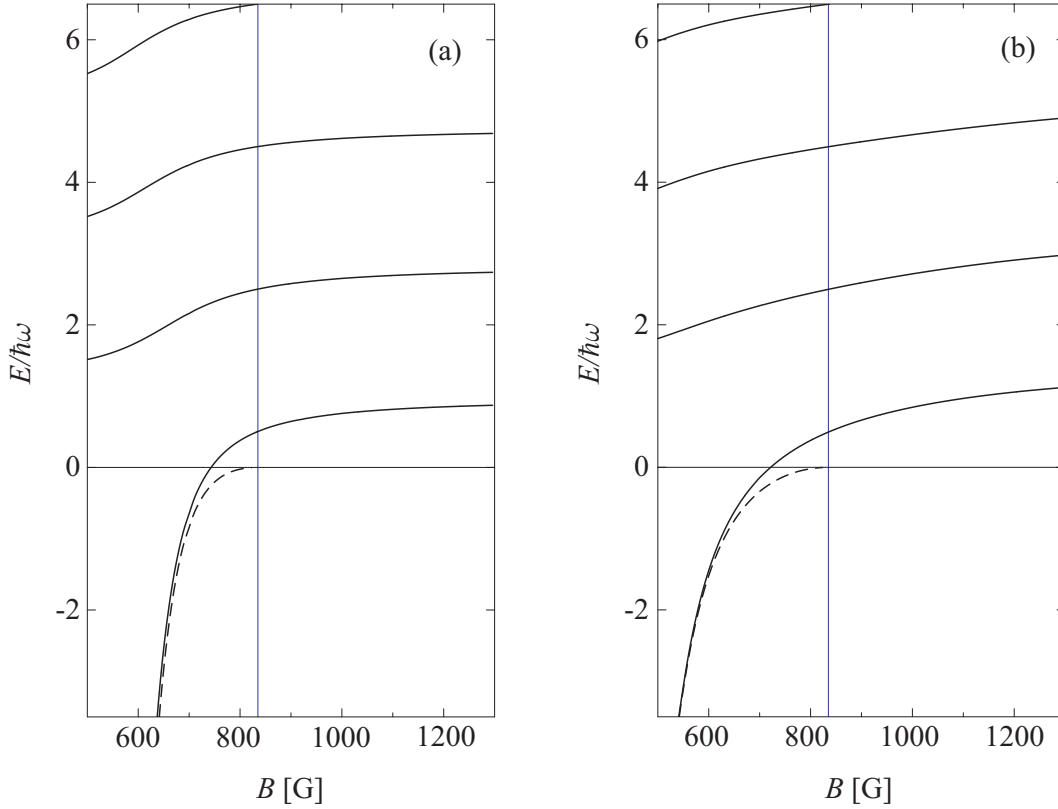
Figure 3. (a) Relative energy levels (solid lines) as a function of the magnetic field B for a system consisting of two ^{6}Li atoms in the hyperfine states $|1\rangle$ and $|2\rangle$ near the Feshbach resonance at 834 G in a harmonic potential of $\omega = 10^6$ s^{-1} with background atom-atom scattering taken into account. The dashed line corresponds to the binding energy of a dressed ^{6}Li$_2$-molecule in the absence of an optical lattice. Note that as the eigenenergy of the dressed molecular ground state with optical lattice (solid line) decreases, it converges to the dressed molecular eigenenergy without optical lattice (dashed line). (b) Similar to panel (a), only this time the background atom-atom scattering is not taken into account. Note that as a result both panels differ significantly.

The difference between equations (61) and (77) in the case of ^{6}Li becomes even clearer when we look at the corresponding wavefunction renormalization factors Z_σ given by equation (48), which are needed for the construction of the effective Hamiltonian given by equation (50). For the calculation of Z_σ we need the molecular self-energy $\hbar\Sigma_{\mathrm{m}}$, which is given by the right-hand side of equation (61) for the case without background atom-atom scattering and by the right-hand side of equation (77) for the case with background atom-atom scattering. In figure 4, the corresponding wavefunction renormalization factors Z_σ are plotted for both cases as a function of the magnetic field B. Here, Z_0 corresponds to the groundstate of the relative on-site two-body Hamiltonian, Z_1 corresponds to the first excited state, and so on. Note that the two-body renormalization factors Z_σ obtained including background interactions (figure 4a), are very different from the factors obtained without background interactions (figure 4b).
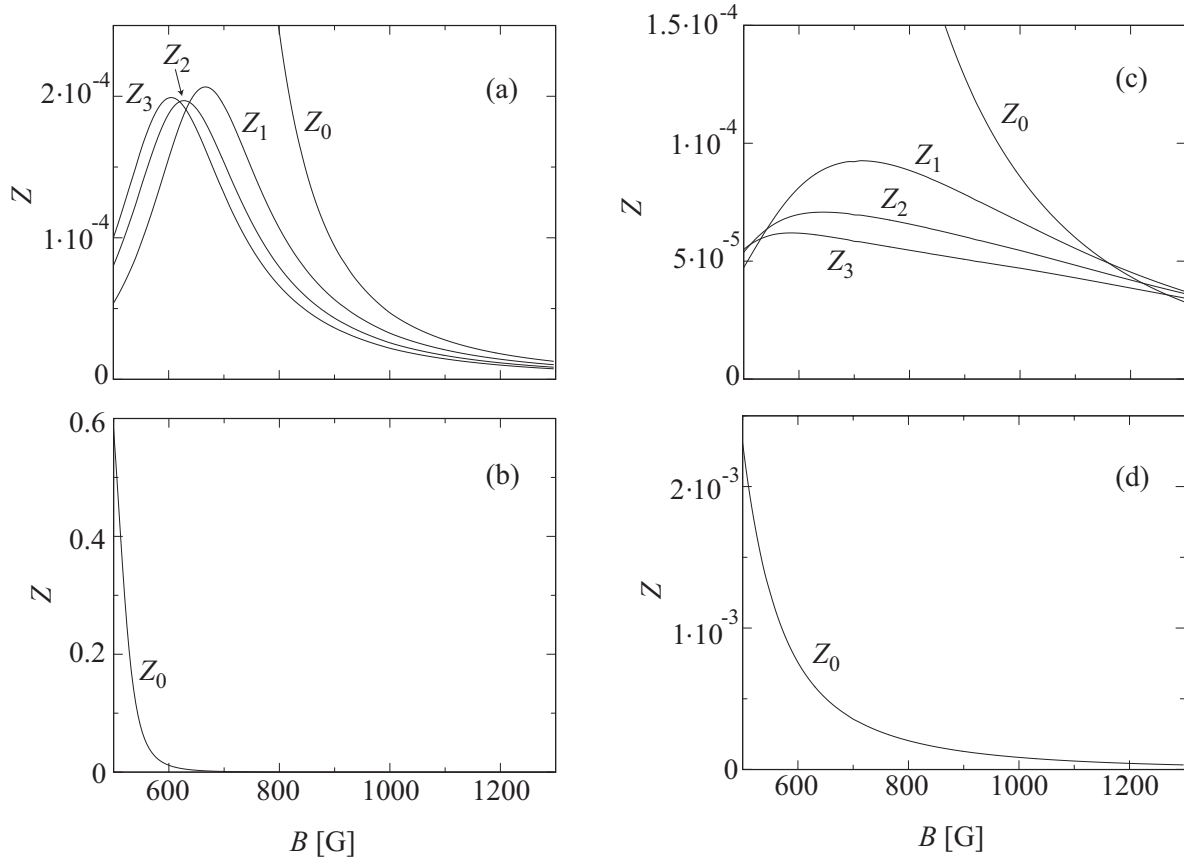
Figure 4. (a),(b) Wavefunction renormalization factors Z_σ for ^{6}Li near the Feshbach resonance at 834 G as a function of the magnetic field B with background atom-atom scattering taken into account. Z_0 is the renormalization factor corresponding to the ground state of the two-body on-site Feshbach problem, Z_1 is the renormalization factor corresponding to the first excited state, and so on. (c),(d) Wavefunction renormalization factors Z_σ for ^{6}Li as a function of the magnetic field B without background atom-atom scattering. Note that the panels on the left differ significantly from the panels on the right.

Also note that these factors are directly experimentally observable as demonstrated by Partridge *et al.* [7]. We thus conclude that background atom-atom scattering plays a significant role for an atomic gas of ^{6}Li atoms in an optical lattice near the Feshbach resonance at 834 G.

4. Conclusion

In summary, we have derived from first principles an effective atom-molecule theory that describes an atomic gas in an optical lattice near a Feshbach resonance. The theory was formulated in the tight-binding limit and incorporated all the relevant two-body physics exactly. The field-theoretical derivation reconfirmed that an atomic gas in an optical lattice near a Feshbach resonance is accurately described by a generalized Hubbard model, as first obtained in ref. [13]. In the original approach of ref. [13] the

generalized Hubbard model was derived in an easier way by starting from a two-body calculation on a single site. Due to the equivalence of both approaches, we used the latter to formulate a way in which to include the background atom-atom scattering into the many-body theory, which has not been done previously. To this end, we showed how to solve exactly the two-channel Feshbach problem for two atoms on a single site including background atom-atom scattering. The solution was applied to ^{6}Li near the experimentally relevant Feshbach resonance at 834 G. Specifically, the two-body on-site energy levels and the wavefunction renormalization factors Z_σ were obtained, which are needed for the generalized Hubbard Hamiltonian describing the many-body physics. As it turned out, the various energy levels and the wavefunction renormalization factors obtained with background interactions taken into account, are significantly different from the energy levels and the renormalization factors obtained without background interactions taken into account. From this we conclude that in the case of ^{6}Li background atom-atom scattering plays an important role and cannot be neglected for an accurate microscopic description of future experiments with atomic lithium in an optical lattice.

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